Low energy states with different symmetries in the t-J model with two holes on a 32-site lattice

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We study the low energy states of the t-J model with two holes on a 32-site lattice with periodic boundary conditions. In contrary to common belief, we find that the state with $d_{x^2-y^2}$ symmetry is not always the ground state in the realistic parameter range $0.2 \leq J/t \leq 0.4$. There exist low-lying finite-momentum p-states whose energies are lower than the $d_{x^2-y^2}$ state when J/t is small enough. We compare various properties of these low energy states at $J/t = 0.3$ where they are almost degenerate, and find that those properties associated with the holes (such as the hole-hole correlation and the electron momentum distribution function) are very different between the $d_{x^2-y^2}$ and p states, while their spin properties are very similar. Finally, we demonstrate that by adding "realistic" terms to the t-J model Hamiltonian, we can easily destroy the $d_{x^2-y^2}$ ground state. This casts doubt on the robustness of the $d_{x^2-y^2}$ state as the ground state in a microscopic model for the high temperature superconductors.

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I. INTRODUCTION

The t-J model was proposed as a microscopic model to describe the low energy physics of high temperature superconductors. It mimics the doped CuO_2 planes found in high temperature superconductors by a system consisting of mobile holes moving in a spin background on a two-dimensional square lattice.[1] One possible mechanism for superconductivity is the Bose-Einstein condensation of "preformed" hole pairs. To see whether this is possible, first we have to understand how the holes interact. It is well-known that a mobile hole causes frustration in the antiferromagnetic spin background. Longer range interaction between the holes must be mediated through the spin distortion they produce. Various studies[2] seem to indicate that in the "realistic" parameter range $J/t \sim 0.3$–0.4, the holes form bound pairs in the $d_{x^2-y^2}$ channel. Theoretically this can be understood as resulting from the magnon exchange interaction which selects the $d_{x^2-y^2}$ channel over others.[3] Alternatively, the density matrix renormalization group (DMRG) approach has been used to work out the spin structure in the vicinity of a hole pair in real space.[4] It was found that by pairing up at a distance of $\sqrt{2}$, the two holes can share the spin frustration and is therefore energetically favorable. This is consistent with the numerical observation[5,6,7] that the holes have the largest probability of being at $\sqrt{2}$ apart. Later it was shown that such pairing of holes at $\sqrt{2}$ arises naturally if the wavefunction has $d_{x^2-y^2}$ symmetry.[8] But in order to firmly establish the role of d-wave hole pairing in the theory of superconductivity, one has to understand how strong and robust the pairing is. In fact numerical study[7] has shown that the binding energy of the d channel is negative but small, and that the holes may not be tightly bound in real space. Recently the question on the robustness of d-wave pairing was addressed by using the anisotropic t-J_z model as the starting point.[9] It concluded that different mechanisms may select states with different symmetries and their competition may destroy the d-wave ground state. This raises doubt on the robustness of the d-wave ground state because it is known that the t-J model alone is not enough to explain fully the hole dynamics of $Sr_2CuO_2Cl_2$ measured by angle-resolved photoemission.[10] In order to reproduce the measured spectral functions, one has to add longer-range hole hopping terms (t', t'' and a three-site hopping term) to the t-J model Hamiltonian.[11,12,13]

Motivated by the above discussion, we study the low energy states of the two-hole t-J model with different symmetries using exact diagonalization (ED). Previous ED studies were mostly performed on square lattices of 16, 20, and 26 sites. Since we are focusing on the symmetry of the wavefunctions, the geometry of the lattice is very important. For example, it is well-known that on the 16-site (4×4) lattice the system has spurious degeneracy at the wavevectors $(\pi/2, \pi/2)$ and $(\pi, 0)$. The 32-site lattice is free from these spurious effects. The $d_{x^2-y^2}$ state of the two-hole model on the 32-site lattice has been studied in Ref. 7. Besides, previous works have indicated that there is a p-wave state whose energy is very close to that of the $d_{x^2-y^2}$ state at realistic values of J/t.[14] The existence of this low energy state casts doubt on the robustness of the $d_{x^2-y^2}$ state as the ground state of the two-hole model. The energy difference is so small that any additional terms in the Hamiltonian may change the ground state from one to another. This cross-over may be realized by adding longer range hopping terms mention above to the t-J model Hamiltonian. Furthermore, it has been shown that such terms favor the p-wave state.[9] This shows that the physics of the low-lying p state may not be irrelevant. Therefore it is important to understand the similarities and differences between the properties of the $d_{x^2-y^2}$ and the p states. In a previous publication[14] we have shown that the hole and current correlations of these two states are very different. In this paper, we will discuss in more detail the low-lying states of the two-hole

model in a larger range of J/t. The properties of these states will be compared at the realistic value of $J/t = 0.3$. Finally, we will demonstrate the effects of longer-range hopping and short-range Coulomb repulsion on the symmetry of the ground state.

II. LOW-LYING STATES WITH DIFFERENT SYMMETRIES

The Hamiltonian of the t-J model is

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} (\tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j), \tag{1}$$

where $\tilde{c}^{\dagger}$ and $\tilde{c}$ are the projected fermion operators, and $n_i \equiv \tilde{c}^{\dagger}_i \tilde{c}_i$ is the fermion number operator. We solve this model with two holes on a 32-site lattice using the standard Lanczos algorithm. To find the low-energy states, we consider subspaces with different rotational symmetries and momenta. We concentrate on the rotational symmetries s, p, and d. States having larger angular momentum usually have higher energy and are not relevant in our study. The momenta of the subspaces we study are $(0,0)$, (π,π) and $(\pi,0)$. The dimensions of the subspaces with s and d symmetries are about 150 million, and that of the subspaces with p symmetry are about 300 million. Most of the calculations are performed on a cluster of commodity personal computers. In subspaces with d symmetry, we achieve a speed of about 4.3 minutes per Lanczos iteration on a 32-node cluster, where each node utilizes a 1 GHz Althon CPU.

The energies of the low-lying states are tabulated in Table I. We are interested in the two-hole binding energy which is defined as

$$E_b = E_{2h} - 2E_{1h} + E_{0h}, \tag{2}$$

where E_{nh} is the energy of the n-hole system. The ground state of the undoped system with energy E_{0h} is a totally symmetric state with momentum $(0,0)$. The ground state of the one-hole system with energy E_{1h} has momentum $(\pi/2, \pi/2)$. E_b is the energy gain of the two-hole system relative to two one-hole systems, and therefore indicates the relative tendency for the two holes to form a bound pair. Keeping in mind that the "realistic" value of J is roughly between $0.2t$ and $0.4t$, we calculate the binding energies in a larger range of J in order to get a clear picture of the crossing-over of the energy levels. Fig. 1 shows E_b of the low-lying states with s, p and d symmetries. The lowest energy state in the subspace with s symmetry is a spin singlet with momentum $(0,0)$. We call this the s state. At small J ($J \leq 0.1t$), this is the ground state. But its energy rises very fast with J and soon changes from the ground state to an excited state. This shows that the s channel is energetically unfavorable and is irrelevant at the realistic parameter $J \sim 0.3t$.

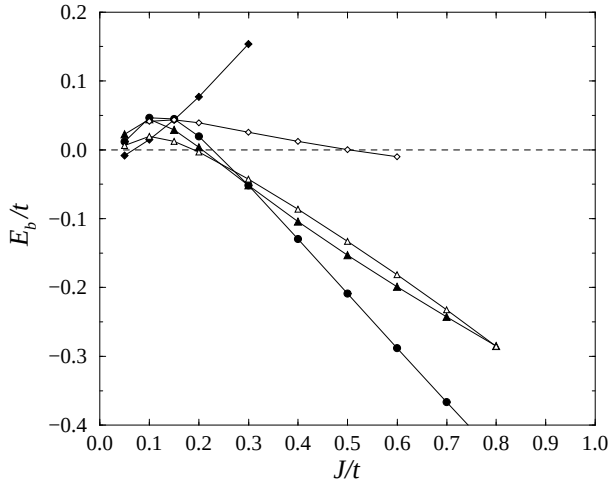

FIG. 1: Two-hole binding energies of the s (solid diamonds), d (solid circles), $p_{(\pi,\pi)}$ (solid triangles), $p_{(\pi,0)}$ (empty triangles), and $p_{(0,0)}$ (empty diamonds) states as defined in the text.

The lowest energy state with d symmetry is a spin singlet with momentum $(0,0)$ and $d_{x^2-y^2}$ symmetry. We call this the d state. This is the same state reported in Ref. 7. At $J > 0.3t$, it is the ground state of the two hole system. Note that the binding energy of this state scales linearly with J when $J > 0.3t$, reflecting the magnetic nature of the hole binding mechanism.[15] Those states with p symmetry are more complicated. In Fig. 1 we show two low energy states with p symmetry. Both of them are two-fold degenerate and are spin singlets. One has momentum (π,π). We call it the $p_{(\pi,\pi)}$ state. The other has momentum $(\pi,0)$. We call it the $p_{(\pi,0)}$ state.[16] In addition, we also show a higher energy p state with zero momentum, which we call the $p_{(0,0)}$ state. This state was mentioned in a previous study using a smaller lattice.[15] Also note that it is a triplet state. Fig. 1 indicates a general trend that as J decreases, the energy of the d state is pushed up faster than the p states. While at $J > 0.3t$ the $p_{(\pi,\pi)}$ and $p_{(\pi,0)}$ states are clearly excited states, the energy levels look quite complicated in the range $0.2t \leq J \leq 0.3t$. Note that the d, $p_{(\pi,\pi)}$ and $p_{(\pi,0)}$ states are almost degenerate at $J = 0.3t$, although the d state is still the ground state. When J is slightly smaller than $0.3t$, it looks like the $p_{(\pi,\pi)}$ state has lower energy than the d state but at $J = 0.2t$, the $p_{(\pi,0)}$ state has the lowest energy among the three. At smaller J, we anticipate more serious finite-size effects. Based on our data only we cannot conclude where the crossing-overs of the energy levels occur, nor whether they exist in the thermodynamic limit. But the fact that the crossing-overs in our system occur at J values within the realistic range is sufficient to cast doubt on the symmetry of the ground state in the two-hole model. Regardless of whether one of the p states actually becomes the ground state at certain range of J, their existence as low-lying states is unquestionable. Furthermore, since the energy levels of these

TABLE I: Energies (E_{2h}/t) of the low-lying states of the two-hole t-J model on a 32-site lattice at different J/t. The s, d, $p_{(0,0)}$, $p_{(\pi,\pi)}$ and $p_{(\pi,0)}$ states are defined in the text. Also shown are the ground state energies E_{1h}/t of the one-hole model. The ground state energy of the undoped model is $E_{0h} = -37.7657342J$.

J/t	E_{1h}/t	E_{2h}/t				
		s	d	$p_{(0,0)}$	$p_{(\pi,\pi)}$	$p_{(\pi,0)}$
0.1	−6.419382	−9.047472	−9.015703	−9.0208259142	−9.017720	−9.042840
0.2	−9.766819	−11.903649	−11.960871	−11.9412605733	−11.976890	−11.983860
0.3	−13.161933	−14.840663	−15.045603	−14.9685556227	−15.045602	−15.036724
0.4	−16.583058		−18.189385	−18.0477851139	−18.163935	−18.146186
0.5	−20.021272		−21.368517	−21.1594455768	−21.312775	−21.292519
0.6	−23.471807		−24.572086	−24.2941123207	−24.483247	−24.465752
0.7	−26.931796		−27.793984		−27.670397	−27.660030
0.8	−30.399375		−31.030391		−30.871142	−30.871578

states are very close, inclusion of farther-than-nearest-neighbor hopping terms or Coulomb repulsion may easily change the ground state from one to another. Therefore we think that they are relevant and warrant detail studies. In the following sections we study in detail the properties of these states at $J = 0.3t$ where they are almost degenerate.

III. REAL SPACE STRUCTURE OF THE HOLE PAIR

Despite the fact that the binding energies of the d and p states at $J = 0.3t$ are very similar and negative, their hole-hole correlations are very different. In Fig. 2 we plot the hole-hole correlation function $C(r) \equiv \langle (1-n_0)(1-n_r)\rangle$. As already discussed in Ref. 7 and also shown in Fig. 2, the holes in the d state attract each other, with $C(r)$ having a maximum at $r = \sqrt{2}$. This has been observed in previous ED studies using smaller lattices.[5,6] Note that the observed attraction cannot be considered to be strong. The probability $P(r)$ of the holes being at $\sqrt{2}$ [$P(\sqrt{2}) = 0.26476$] and $\sqrt{5}$ [$P(\sqrt{5}) = 0.25037$] are almost the same.[17] The root-mean-square separation of the hole pair is $r_{\rm rms} \equiv \sqrt{\langle r^2\rangle} = 2.05865$. Compared to the $r_{\rm rms}$ of two uncorrelated holes in this lattice, which is 2.38273, the hole pair in the d state is not tightly bound. This is consistent with its barely negative E_b. On the contrary the holes in both p states seem to be mutually repulsive despite the negative E_b. Their $r_{\rm rms}$ are 2.53755 and 2.53500 respectively, which are significantly larger than that of the d state. This shows that the hole pairs in the $p_{(\pi,\pi)}$ and $p_{(\pi,0)}$ states are unbound.

The spatial correlation of the hole pairs described above can be understood in terms of the nearest neighbor spin correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle$ at fixed hole configuration. This analysis was first carried out on a two-hole bound state using the technique of density matrix renormalization group,[4] and later by ED.[8] Fig. 3 shows our result for the d state on a 32-site lattice. The most intriguing feature is the existence of a strong next-nearest neighbor (i.e. across the diagonal of a square plaquette) singlet

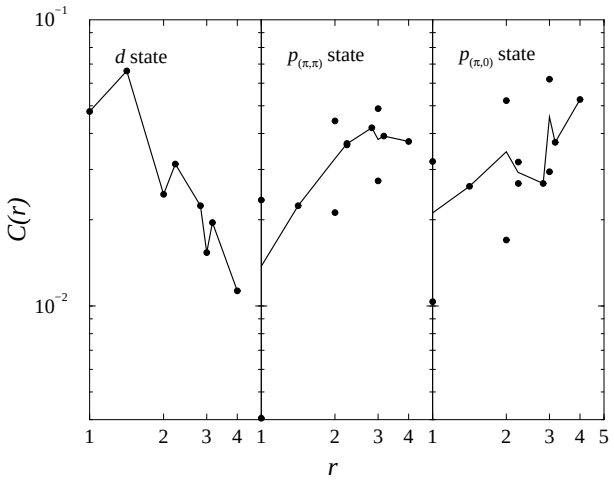

FIG. 2: Hole-hole correlation function $C(r)$ of the d and p states at $J = 0.3t$. Due to the lack of the rotational symmetry C_4 (i.e., a rotation by $\pi/2$) in the p states, there may be two inequivalent points at the same r. In this case their values are indicated by the symbols and the solid line joins their mean values.

bond in between two holes when they are at distance $\sqrt{2}$ apart. This is shown in Fig. 3a. It has been argued[4] that such singlet bond increases the hopping overlap between different hole configurations – when a hole hops this singlet bond becomes a strong nearest neighbor bond, and therefore is energetically favorable. But such singlet bond between two spins in the same sublattice causes spin frustration around the plaquette. Therefore the two holes tend to stay at next-nearest-neighbor distance in order to share the frustrating singlet bond. This explains why the holes are more likely to be found at distance $\sqrt{2}$ as shown in Fig. 2. When the holes are farther part as shown in Fig. 3b, a diagonal singlet bond still exists in the immediate vicinity of each hole, although it is weakened compared to the one in Fig. 3a. Besides, across each hole there is another strong singlet bond between two spins at a distance of 2. These two singlet bonds encourage the holes to hop towards each other because doing so will create two strong nearest-neighbor singlet

bonds. Such characteristic is retained in the other hole configurations shown in Fig. 3, although the strength of the singlet bonds weaken quickly as the holes move farther apart. Note that this set of hole configurations consistently have larger hole correlation $C(r)$ as shown in Fig. 2. For the other hole configurations where the holes are along the x or y directions, the characteristics of the spin correlations around the holes are very different. Two of these hole configurations are shown in Fig. 4. When the holes are at nearest neighbor distance (Fig. 4a), there are two strong nearest neighbor singlet bonds immediate above and below the hole pair. When one hole hops to become the hole configuration in Fig. 3a, one of these singlet bonds becomes the strong diagonal single bonds, and the other remains as a strong nearest neighbor bond. We can see the reminiscence of this bond on the four sides of the diagonal bond in Fig. 3a. Such hopping is strongly preferred as shown in the kinetic energy plot of Fig. 5. When the holes are at $\sqrt{2}$ apart, the hopping energy along the four directions are significantly larger. When the holes are far apart (Fig. 4b), the spin correlation around the hole does not seem to possess any special feature. The hole hopping energy also decreases rapidly. However, contrary to a previous study,[4] when the holes are close to each other, we do not see evidence for dimerization in the vicinity of the holes. In Fig. 6 we show the spin correlation relative to the undoped value. Except at the immediate vicinity of the holes, the spin correlation is rather unaffected and there is no clear evidence of dimerization.

Next let us consider the low-energy state $p_{(\pi,\pi)}$. As already pointed out before,[4] the spin correlation in the vicinity of a pair of near-by holes discussed above provides a mechanism for hole binding. It has also been argued that such spin correlation is a result of the $d_{x^2-y^2}$ symmetry of the wavefunction.[8] Then it is reasonable to expect that in wavefunctions with other symmetries, such mechanism for hole binding is missing and the holes may be unbound. Fig. 7 seems to support this. When we compare the d and $p_{(\pi,\pi)}$ wavefunctions in the same subspace where the holes are at $\sqrt{2}$ apart (Fig. 3a and 7a), we find striking differences in the spin correlation. The strong diagonal singlet bond between the holes found in the d state does not exist in the $p_{(\pi,\pi)}$ state. The binding mechanism discussed above is therefore missing in the $p_{(\pi,\pi)}$ state. This causes the probability for the hole pairs at $\sqrt{2}$ apart to be small, as evident from Fig. 2. On the other hand, when the holes are far apart we observe a strong singlet spin pair across each hole (Fig. 7b). It becomes a strong nearest neighbor singlet bond when the hole hops, thus increasing the overlap with other hole configurations and making it a preferred hole configuration. This feature is missing in the d state (Fig. 3d), where large hole separations are not preferred. This explains the repulsive nature of the holes in the $p_{(\pi,\pi)}$ state as shown in Fig. 2. Note that this interpretation is also consistent with the hole hopping energy as shown in Fig. 5b. The hopping

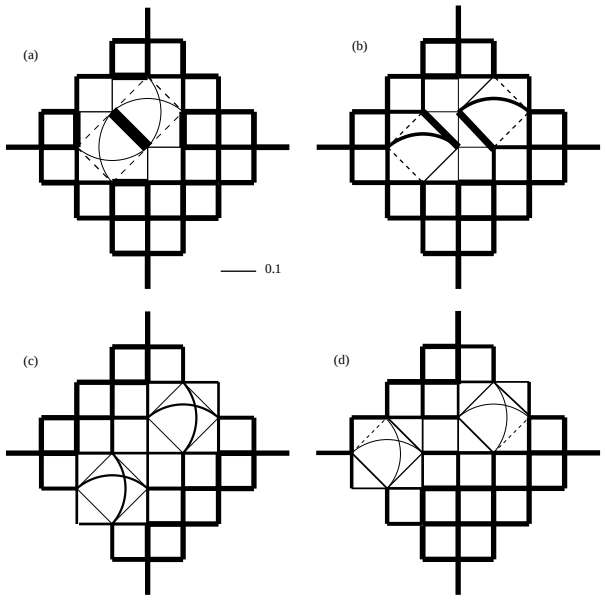

FIG. 3: Spin correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ in the d state at $J = 0.3t$. The two empty lattice points in each diagram are the locations of the holes. Only nearest neighbor spin correlations are shown except in the vicinity of the holes where the correlations between spins at $\sqrt{2}$ and 2 apart are also shown. The width of the line joining two spins i and j is proportional to $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle / P(r)$, where $P(r)$ is the probability of finding the holes at the relative locations as shown. Solid and broken lines mean $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ are negative and positive respectively.

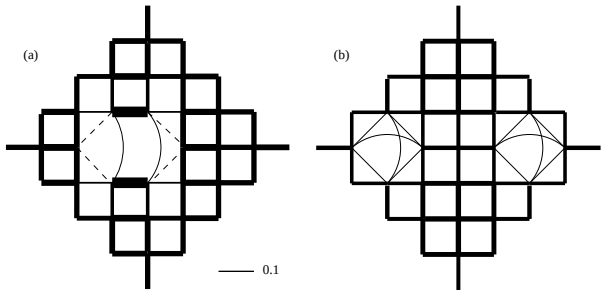

FIG. 4: Same as Fig. 3 but for different hole configurations.

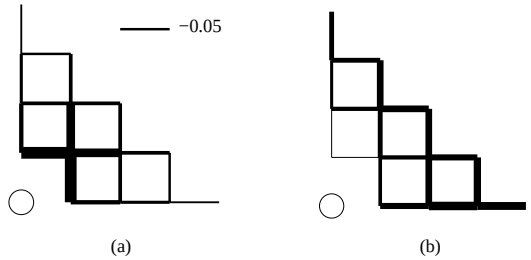

FIG. 5: The hole hopping energy $\langle \tilde{c}_i^\dagger \tilde{c}_j \rangle$ when the other hole is fixed at the location indicated by an empty circle, in (a) the d state and (b) the $p_{(\pi,\pi)}$ state, both at $J = 0.3t$. Only a quarter of the lattice is shown. Values at other nearest neighbor pairs $\langle ij \rangle$ can be found by using the symmetry of the lattice.

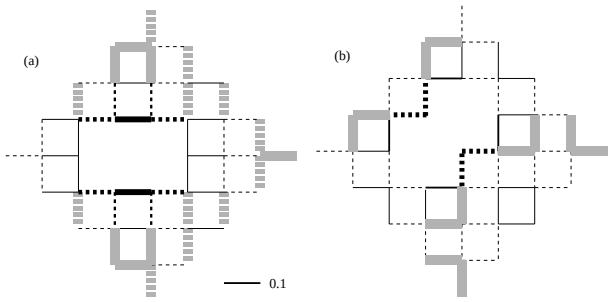

FIG. 6: The spin correlation relative to the undoped value, $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle / P(r) - \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{\rm undoped}$, of the d state at $J = 0.3t$. $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{\rm undoped} = -0.34009$. Solid and broken lines mean that the singlet correlation are enhanced (more negative) and suppressed (less negative) respectively relative to $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{\rm undoped}$. Only nearest neighbor correlations are shown. Those thick shaded lines mean that their values are too small to be shown in this scale, with magnitude smaller than 0.02. Their thickness do not represent the magnitude. They are drawn to show the sign of their values only.

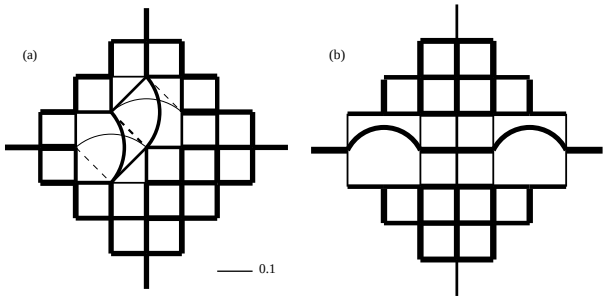

FIG. 7: Same as Fig. 3 but for the $p_{(\pi,\pi)}$ state at $J = 0.3t$. The scale of the line width is also the same as in Fig. 3.

energy is larger when the holes are farther apart.

IV. MOMENTUM SPACE DISTRIBUTION

Fig. 8 shows the electron momentum distribution function (EMDF), defined as $\langle n_{\mathbf{k}\sigma} \rangle \equiv \langle \tilde{c}^\dagger_{\mathbf{k}\sigma} \tilde{c}_{\mathbf{k}\sigma} \rangle$, for the three low energy states. Since in the two-hole model $\langle n_{\mathbf{k}\uparrow} \rangle = \langle n_{\mathbf{k}\downarrow} \rangle$, we will leave out the spin index σ. This quantity demonstrates another striking difference between the d and p states. Previous works[18] have shown that the general shape of $\langle n_{\mathbf{k}} \rangle$ is irrelevant to the structure of the hole pair. This is evident from the fact that in the two-hole model, $\Delta n \equiv (\langle n_{(0,0)} \rangle - \langle n_{(\pi,\pi)} \rangle)$ is roughly the same as $(\Delta n^{1h}_\uparrow + \Delta n^{1h}_\downarrow)$.[19] Note that this is true for all the three low-energy states. Nevertheless, those $\mathbf{k}$ along the magnetic Brillouin zone boundary [$(\pi, 0)$ to $(0, \pi)$] are important in reflecting the structure of the bound state.[7] The deviation of the EMDF from the undoped value, $\langle n_{\mathbf{k}} \rangle - \frac{1}{2}$, represents the hole weight at that $\mathbf{k}$. As already pointed out in Ref. 7 and shown in Fig. 8, $\langle n_{\mathbf{k}} \rangle$ of the d state along the magnetic Brillouin zone boundary has a maximum at $(\pi/2, \pi/2)$, and minimum somewhere between $(\pi/2, \pi/2)$ and $(\pi, 0)$. Note that in the d state $\langle n_{\mathbf{k}} \rangle$ is symmetric about the line from $(0, 0)$ to (π, π), and in the 32-site lattice the two minima in the first quadrant of the Brillouin zone are at $(3\pi/4, \pi/4)$ and $(\pi/4, 3\pi/4)$. On the contrary, in the p states the minimum of $\langle n_{\mathbf{k}} \rangle$ along the magnetic Brillouin zone boundary is at $(\pi/2, \pi/2)$. Note that the symmetry of the d state requires the hole weight at $(\pi/2, \pi/2)$ to be zero. Hence its $\langle n_{(\pi/2,\pi/2)} \rangle$ deviates from the undoped value of $\frac{1}{2}$ by a minimal value of 0.0064. Such restriction is lifted in the p states and in fact $\langle n_{\mathbf{k}} \rangle$ shows that their hole weight is a maximum at $(\pi/2, \pi/2)$. This feature resembles a hole pocket at $(\pi/2, \pi/2)$. The fact that the EMDF of the p states have dimples at momenta corresponding to the single-particle ground state leads us to think that some form of rigid band filling approximation works in the p states but not in the d state. This can be accounted for by their different hole-hole correlations in real space. When the holes are farther apart, the overlap in the spin distortions they produce is smaller. Therefore the state can be better approximated by some combination of the single-hole quasiparticle states, thus making the rigid band filling model a better approximation.

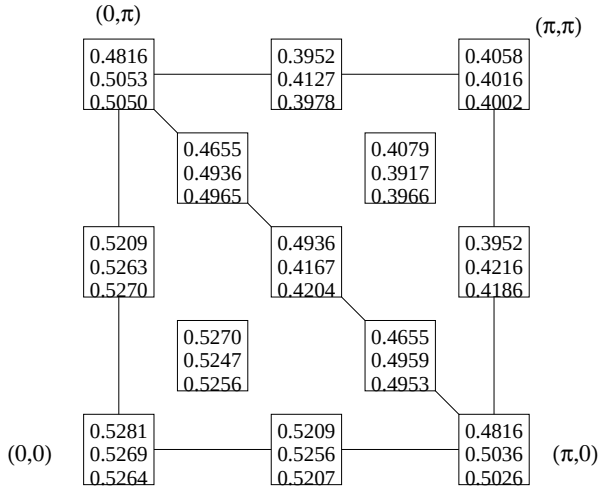

FIG. 8: EMDF of the low energy states. Each box represents an allowed momentum $\mathbf{k}$. The three numbers inside each box, from top to bottom, are $\langle n_{\mathbf{k}} \rangle$ of the d, $p_{(\pi,\pi)}$ and $p_{(\pi,0)}$ states at $J = 0.3t$. Only the first quadrant of the Brillouin zone is shown. $\langle n_{\mathbf{k}} \rangle$ in other quadrants can be constructed by using the symmetry of the Brillouin zone.

V. SPIN CORRELATION

Next we turn to the spin properties of the three low energy states at $J = 0.3t$. We first study the static structure factor $S(\mathbf{k})$ and the spin correlation function

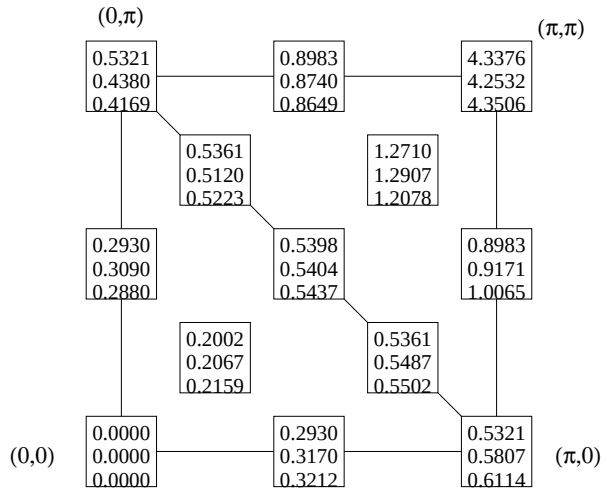

FIG. 9: Same as Fig. 8 but for the static structure factor $S(\mathbf{k})$.

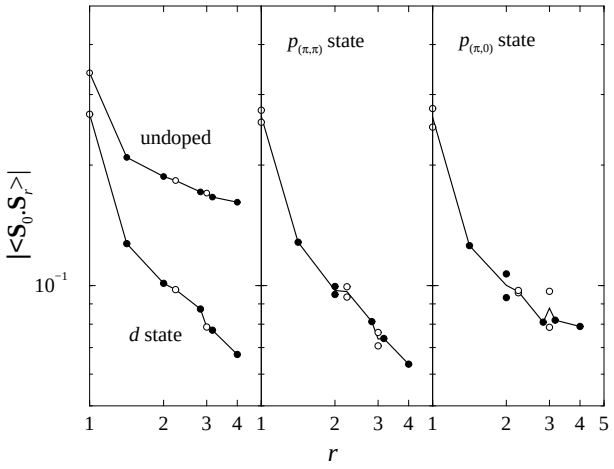

FIG. 10: Spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$ of the three low energy states at $J = 0.3t$. Also shown is the same result on the ground state of the undoped system on the same lattice. Filled and empty circles represent positive and negative correlations respectively.

$\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$. They are related by

$$S(\mathbf{k}) = \sum_r e^{-i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle. \quad (3)$$

Fig. 9 shows the static structure factors. All three states show strong characteristics of a Néel state – $S(\mathbf{k})$ strongly peaks at (π, π). It is interesting to note that while those properties associated with the holes are very different between the p and d states, their static structure factors are very similar. As far as the spin property is concerned, the effect of the holes added to the system is to weaken the Néel order only, with no qualitative change. This is also indicated in the spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$ in Fig. 10. It is obvious that the spin correlations of the d and $p_{(\pi,\pi)}$ states have very similar behavior. If we fit a power law to the data points at $r \geq 2$, we find that the spin correlation decays as $r^{-0.61}$ in the d state and $r^{-0.68}$ in the $p_{(\pi,\pi)}$ state. They are to be compared to the spin correlation of the undoped ground state on the same 32-site lattice which decays as $r^{-0.25}$. The spin correlation of the $p_{(\pi,0)}$ state seems to be of a bit longer range and cannot be fitted satisfactorily by a power law. However, the difference does not show up significantly in the static structure factor.

In the semi-classical theory of Shraiman and Siggia, a mobile hole produces long-range dipolar distortion in the spin background.[20] A consequence is that the holes tend to stay away to minimize the overlap of the spin distortion they produce, resulting in dimples in the EMDF at momenta corresponding to the single-hole ground state. As discussed in the last paragraph of the previous section, the p states seem to fit this scenario better than the d state. Another consequence of the semi-classical theory is that in the presence of a small number of holes, the system may be unstable towards the spiral phase.[21] Therefore it is interesting to compare the tendency of the d and p states to have spiral order. A consequence of the spiral phase is that the maximum of $S(\mathbf{k})$ will shift away from $\mathbf{k} = (\pi, \pi)$. As shown in Fig. 9, we do not see such pattern in any of the three low-energy states. However, the shift in $\mathbf{k}$ may be too small to be detected in our finite lattice with discrete $\mathbf{k}$. In previous ED studies of the t-J model on smaller lattices, the shift in $S(\mathbf{k})$ was not observed until the doping level is much larger.[22,23] On the other hand, experiments has demonstrated incommensurability in the magnetic fluctuation.[24] Therefore one should not look for long range order that exists in the thermodynamic limit, but should instead look for short-range spiral order. For this reason we calculate the twist order parameter which is defined as

$$\boldsymbol{\chi}_i^t = \mathbf{S}_i \times (\mathbf{S}_{i+\mathbf{x}} + \mathbf{S}_{i+\mathbf{y}}). \quad (4)$$

Fig. 11 shows $\langle \boldsymbol{\chi}_0^t \cdot \boldsymbol{\chi}_r^t \rangle$ in the three low energy states. The short range behavior of this correlation function is very similar in the d and $p_{(\pi,\pi)}$ states. In the $p_{(\pi,0)}$ state it seems to decay faster. We find no enhancement in the short range spiral order in the p states relative to the d state, and the correlation functions are very small in all three states. The susceptibility, defined as $\langle \frac{1}{N^2} | \sum_r \boldsymbol{\chi}_r^t |^2 \rangle$, are 0.02519, 0.02296, and 0.02492 for the d, $p_{(\pi,\pi)}$ and $p_{(\pi,0)}$ states respectively. These are to be compared to the corresponding value of the undoped model on the same lattice, 0.02052.

VI. ROBUSTNESS OF THE $d_{x^2-y^2}$ GROUND STATE

Fig. 1 shows that in our system the energies of the d and p states are very close at $J \sim 0.3t$. This casts doubt on whether the d state is always the ground state of the two-hole model in the physically relevant range of

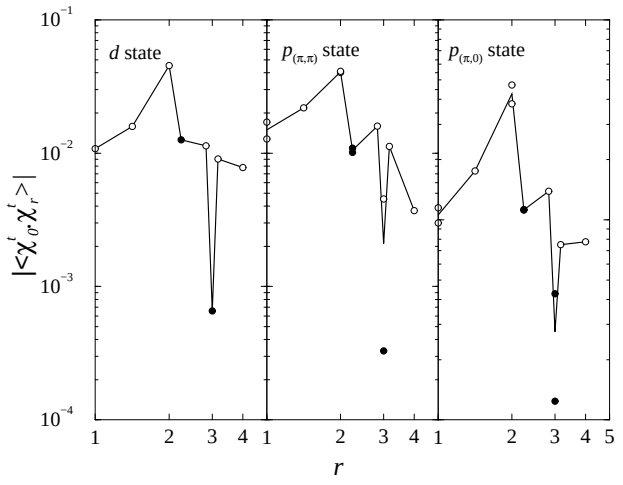

FIG. 11: Same as Fig. 10 except for the spiral spin correlation $\langle \chi_0^t \cdot \chi_r^t \rangle$.

J. Furthermore, the small energy difference means that including additional terms in the t-J model Hamiltonian may have profound effect on the selection of the ground state. This raises the question on the robustness of the d state as the ground state. In this section we discuss the effect on the energy levels when two kinds of terms are added to the t-J model.

As pointed out in Ref. 8, a small size bound pair may be destroyed by a realistic short-range Coulomb repulsion. On a two-leg ladder, the authors have shown that the bound pair disappears around $V \sim 4J$, where V is the nearest neighbor Coulomb repulsion. Recently Coulomb repulsions are found to enhance the staggered orbital current on a two-leg ladder.[25] On a two-dimensional lattice, such staggered current has been found even without Coulomb repulsions.[14,26] Adding them to the two-dimensional model may do more than just pushing the holes apart. The repulsions should weaken hole binding and raise the energy of the d state. But in the p states, the effect is less significant because the holes are already far apart. As a result one would expect short-range Coulomb repulsions to favor the p states to the d state. Here we add two repulsion terms V_1 and V_2 to the t-J Hamiltonian. They are repulsions between two holes at 1 and $\sqrt{2}$ apart respectively. To test the stability of the $d_{x^2-y^2}$ ground state, we choose to use the values $V_1 = 0.6t$, $V_2 = 0.3t$. The binding energies of the three states are shown in Fig. 12 as a function of J/t. As expected, the binding energy of the d state is pushed up more than that of the p states. At $J = 0.3t$, only E_b of the $p_{(\pi,\pi)}$ state is barely negative. In the range we study, $0.2t \leq J \leq 0.8$, the $p_{(\pi,\pi)}$ state has the lowest energy. This calculation shows that even a small Coulomb repulsion will destroy the two-hole bound state and select the p state as the ground state.

It is know that in order to reproduce the single hole dispersion observed experimentally,[10] one has to add longer range hole hopping terms t' and t'' to the t-J model.[12,13]

TABLE II: Energies E_{2h} and binding energies E_b of the lowest energy states with different symmetries of the two-hole t-t'-t''-J model with $J = 0.3t$, $t' = -0.3t$, and $t'' = 0.2t$. Ground state energy E_{1h} of the one-hole model is $-13.716526t$.

symmetry	momentum	spin	E_{2h}/t	E_b/t
d	(0, 0)	0	−15.588993	0.51434
s	(0, 0)	0	−16.074058	0.02927
p	(0, 0)	1	−16.080823	0.02251
p	(π,0), (0, π)	0	−16.109653	−0.00632
p	(π, π)	0	−16.164444	−0.06111

These terms are relevant here for two reasons. First the magnitude of these terms, $t' = -0.3t$ and $t'' = 0.2t$,[13] are larger than the energy difference between the d and p states at $J = 0.3t$. Therefore they may have serious effect on the low-lying energy levels. Second, it has been argued that the form of single-hole dispersion resulting from the t' and t'' terms favors the p state.[9] In Ref. 13, three-site hopping terms are also included in addition to t' and t'' in order to reproduce the spectral functions measured experimentally. However, if we just want to reproduce the single hole dispersion, it will be suffice to include the t' and t'' terms only. Table II shows the lowest energy state in different symmetry subspaces when $t' = -0.3t$ and $t'' = 0.2t$ are included in the t-J model at $J = 0.3t$. We can see that the structure of the low-lying energy levels is seriously affected. First, the energy of the d state is pushed up by a lot compared to other states. Its energy is now even higher than an s and a (triplet) p state. Note that in the t-J model these two states have higher energies than the d state (see section II). Nevertheless, their binding energies are positive. Only the two singlet p states have negative binding energies. The p state with momentum (π, π) now becomes the ground state. Note that its binding energy does not differ too much from that of the t-J model as shown in Fig. 1, which is $-0.05146t$.

VII. CONCLUSION

We tried to map out the low-lying states of the t-J model with two holes on a 32-site square lattice at various J/t. While previous studies have focussed on finding the critical J/t where hole binding is lost, we concentrate on the symmetry of the ground state at different J/t. We find that at large J/t, the ground state has $d_{x^2-y^2}$ symmetry as reported before. But there are low-lying states with p symmetry whose energies come closer to the ground state as J/t decreases. At $J/t < 0.3$ one of these p-wave state becomes the ground state. We note that these p-wave states have non-zero momenta. Previous numerical works have revealed similar finite momentum states. But calculations carried out on lattices smaller than 32 sites are biased by their geometry. As a result, these finite momentum p states have not re-

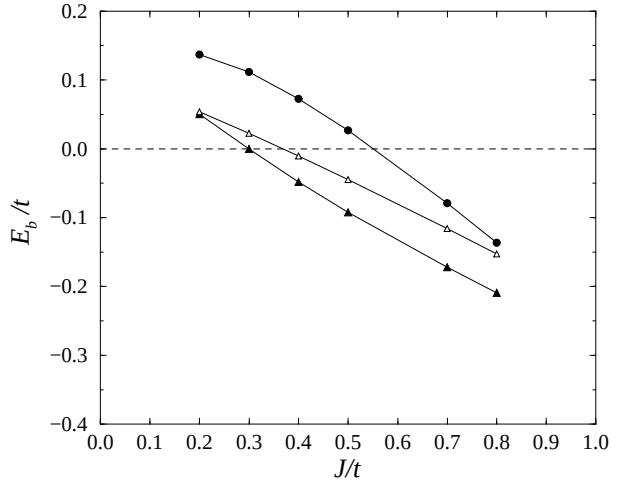

FIG. 12: Same as Fig. 1 except that the Coulomb repulsion terms $V_1 = 0.6t$ and $V_2 = 0.3t$ are added to the t-J model Hamiltonian. The states shown are d (circles), $p_{(\pi,\pi)}$ (solid triangles) and $p_{(\pi,0)}$ (empty triangles).

ceived much attention. Nevertheless, a similar cross-over in the symmetry of the ground state from d to p symmetry has been reported in a series expansion study of the t-J model.[27] There the cross-over was found to be at $J/t \sim 0.4$, which is quite close to our value of $J/t \sim 0.3$. This cross-over was also observed in the anisotropic t-J_z model.[9,27] Although finite-size effects prevent us from concluding definitely whether this cross-over exists in the thermodynamic limit, the fact that it occurs within the parameter range of interest make us feel that the p states are relevant to the low energy physics of the t-J model. Further investigation reveals qualitative differences and similarities in the properties of the p and d states. Perhaps the most intriguing is the difference in their hole properties. The holes are mutually attractive in the d state, but are repulsive in the p states. The spin structure in the vicinity of the holes provides an intuitive explanation of the contrasting behaviors. And as a result of this, the electron momentum distribution functions are also very different. While the EMDF of the d state shows no sign of hole pockets, that of the p states clearly have dimples at $(\pi/2, \pi/2)$. Such hole properties suggest that the rigid-band filling assumption should work better in the p than in the d state, if it works at all. And in the framework of the semi-classical theory,[21] one would expect the p states to have stronger tendency to show spiral spin order than the d state. However, we do not find any enhancement in the short-range spiral spin correlation in the p states over the d state. In fact the spin correlations of the d and p states are very similar and show signals of the Néel state.

We have also demonstrated that the $d_{x^2-y^2}$ ground state is not robust. It can be destroyed easily by including realistic terms to the t-J model Hamiltonian. Both the short-range Coulomb repulsion and longer range hopping terms (t' and t'') favor the p state with momentum (π, π) as the ground state. This shows that hole pairing in the $d_{x^2-y^2}$ channel may not be a generic feature of the t-J model. There is a competing p state which has no hole pairing. The implication of our result is that the symmetry of the two-hole ground state of the t-J model is yet to be determined. This is in contrary to a recent numerical study[28] which concludes that pairing in the $d_{x^2-y^2}$ channel is a robust property of the t-J model.

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$N_E(r)C(r)$, where $N_E(r)$ is the number of equivalent pairs at the same r apart in this finite cluster.

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